

RECEIVED  
JAN 17 2007

2007 FEB 28 AM 7:36

201-16554D

# I U C L I D

## Data Set

**Existing Chemical** : ID: 68515-48-0  
**CAS No.** : 68515-48-0  
**EINECS Name** : 1,2-Benzenedicarboxylic acid, Di-C8-C10 Branched Alkyl Esters, C9 Rich  
**EC No.** : 271-090-9  
**Molecular Weight** : 418  
**Structural Formula** : c(ccc1C(=O)OCC(C)CCC(C)CC)cc1C(=O)OCC(C)CCC(C)CC  
**Molecular Formula** : C26O4H42

**Producer related part**  
**Company** : ExxonMobil Biomedical Sciences Inc.  
**Creation date** : 08.05.2006

**Substance related part**  
**Company** : ExxonMobil Biomedical Sciences Inc.  
**Creation date** : 08.05.2006

**Status** :  
**Memo** : ACC Phthalate Ester Panel HPV Testing Group

**Printing date** : 07.12.2006  
**Revision date** :  
**Date of last update** : 07.12.2006

**Number of pages** : 35

**Chapter (profile)** : Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10  
**Reliability (profile)** : Reliability: without reliability, 1, 2, 3, 4  
**Flags (profile)** : Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE),  
Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

## 1.0.1 APPLICANT AND COMPANY INFORMATION

## 1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

## 1.0.3 IDENTITY OF RECIPIENTS

## 1.0.4 DETAILS ON CATEGORY/TEMPLATE

- Comment** : This chemical is not a member of the High Molecular Weight Phthalate Esters subcategory but its data are being used to support a hazard assessment of the subcategory. The subcategory includes eleven CAS numbers (see Freetext Remark).
- Remark** : This chemical is not a member of the High Molecular Weight Phthalate Esters subcategory but its data are being used to support a hazard assessment of the subcategory. The subcategory includes the following eleven CAS numbers:  
68648-93-1 1,2-benzenedicarboxylic acid, mixed decyl and hexyl and octyl diesters (610P)  
117-84-0 1,2-benzenedicarboxylic acid, dioctyl ester (DOP)  
16883-83-3 1,2-Benzenedicarboxylic acid, benzyl 3-hydroxy- 1-isopropyl-2,2-dimethylpropyl ester isobutyrate (B84P)  
68515-40-2 1,2-benzenedicarboxylic acid, benzyl C7-9 branched and linear alkyl (B79P)  
68515-45-7 1,2-benzenedicarboxylic acid, dinonyl ester, branched and linear (DNP)  
68515-43-5 1,2-Benzenedicarboxylic acid, di-C9-11-branched and linear alkyl esters (911P)  
84-77-5 1,2-benzenedicarboxylic acid, didecyl ester (DDP)  
3648-20-2 1,2-benzenedicarboxylic acid, diundecyl ester (DUP)  
85507-79-5 1,2-benzenedicarboxylic acid, di (C11) ester, branched and linear (DinUP)  
111381-91-0 1,2-benzenedicarboxylic acid (C9, C11) ester, branched and linear (Din911P)  
68515-47-9 1,2-benzenedicarboxylic acid, di-C11-14-branched alkyl esters, C13 rich (DTDP)

The phthalate esters comprise a family of chemicals synthesized by esterifying phthalic anhydride with various alcohols in the presence of an acid catalyst. Phthalate esters are all 1,2-benzenedicarboxylic acids with side chain ester groups ranging from C1 to approximately C13. The structural characteristics of the ester side chains affect both the physical/chemical and biological properties of phthalate esters.

Phthalate esters are generally clear to yellow, oily liquids with high boiling ranges (>250°C) and low vapor pressures; properties which contribute to their high physical stability. They are readily soluble in most organic solvents and miscible with alcohol, ether and most oils. The aqueous solubility of phthalate esters is inversely related to their molecular weights. Lower molecular weight phthalates exhibit slight to moderate water solubility, whereas, higher molecular weight phthalates exhibit very low solubility.

The phthalate esters were subdivided into three subcategories based on

## 1. General Information

Id 68515-48-0  
Date 07.12.2006

their physicochemical and toxicological properties. The phthalate esters in this subcategory, High molecular weight phthalates, are produced from alcohols with straight-chain carbon backbones of >C7 or a ring structure.

Eleven of the U.S. HPV chemicals fall into this subcategory, which includes phthalates containing linear and branched diheptyl, dioctyl, dinonyl, didecyl, diundecyl, and ditridecyl alkyl groups. This subcategory also includes phthalates that can contain a benzyl group. Data for this subcategory were supplemented with published information on other phthalate esters currently being assessed under the OECD SIDS program, including di-isononyl (DINP) and di-isodecyl (DIDP) phthalate.

High molecular weight phthalates are used nearly exclusively as plasticizers of PVC. They are very insoluble in water, and have a very low vapor pressure. The extant database demonstrates that these substances have few biological effects.

06.06.2006

### 1.1.0 SUBSTANCE IDENTIFICATION

#### 1.1.1 GENERAL SUBSTANCE INFORMATION

Purity type	:	
Substance type	:	organic
Physical status	:	liquid
Purity	:	> 99.7 % w/w
Colour	:	
Odour	:	
Remark	:	C8-C10 branched alkyl ester, C9 rich, with an average of 9.2 carbons per alkyl chain.

06.07.2006

#### 1.1.2 SPECTRA

### 1.2 SYNONYMS AND TRADENAMES

### 1.3 IMPURITIES

### 1.4 ADDITIVES

### 1.5 TOTAL QUANTITY

#### 1.6.1 LABELLING

#### 1.6.2 CLASSIFICATION

## **1. General Information**

Id 68515-48-0

Date 07.12.2006

### **1.6.3 PACKAGING**

### **1.7 USE PATTERN**

#### **1.7.1 DETAILED USE PATTERN**

#### **1.7.2 METHODS OF MANUFACTURE**

### **1.8 REGULATORY MEASURES**

#### **1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES**

#### **1.8.2 ACCEPTABLE RESIDUES LEVELS**

#### **1.8.3 WATER POLLUTION**

#### **1.8.4 MAJOR ACCIDENT HAZARDS**

#### **1.8.5 AIR POLLUTION**

#### **1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES**

### **1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS**

### **1.9.2 COMPONENTS**

### **1.10 SOURCE OF EXPOSURE**

### **1.11 ADDITIONAL REMARKS**

### **1.12 LAST LITERATURE SEARCH**

### **1.13 REVIEWS**

## 2. Physico-Chemical Data

Id 68515-48-0

Date 07.12.2006

### 2.1 MELTING POINT

**Value** : -48 °C  
**Decomposition** : no, at °C  
**Sublimation** : no  
**Method** : other: calculated  
**Year** :  
**GLP** :  
**Test substance** : other TS: 1,2-benzenedicarboxylic acid, Di-C8-C10 Branched Alkyl Esters, C9 Rich (CAS No. 68515-48-0)

**Remark** : Physicochemical data for 18 commercial phthalate esters from various sources including the public literature, manufacturing specifications, and handbook values were evaluated by an industry peer review process. Valid values were identified and presented in a phthalate ester environmental fate, peer reviewed publication. These data including the values for melting point represent the definitive and currently accepted physicochemical database for selected phthalate esters including diundecyl phthalate. There were no data on purity. Identified data sources included:

Howard P, Banerjee S and Robillard K (1985). Measurement of water solubilities, octanol/water partition coefficients and vapor pressures of commercial phthalate esters. Environ. Tox. Chem 4, 653-661.

Howear P (1989). Handbook of Environmental Fate and Exposure Data for Organic Chemicals: Vol I. Large Production and Priority Pollutants. Lewis Publishers, Inc., Chelsea, MI, USA.

Sears J and Turchette N (1982). Plasticizers, In: Kirk-Othmer Encyclopedia of Chemical Technology, Eds. Mark H, Othmer D, Overberger C and Seaborg G. Vol. 18, 3rd Edition. John Wiley and Sons, New York, NY, USA.

**Test substance** : 1,2-benzenedicarboxylic acid, Di-C8-C10 Branched Alkyl Esters, C9 Rich (CAS No. 68515-48-0)

**Reliability** : (2) valid with restrictions  
Although the original reference was not retrieved and reviewed for quality, this robust summary has a reliability rating of 2 because the data are from a peer reviewed database.

**Flag** : Critical study for SIDS endpoint

06.06.2006

(23)

**Value** : 115 °C  
**Decomposition** : no, at °C  
**Sublimation** : no  
**Method** : other: calculated  
**Year** :  
**GLP** :  
**Test substance** : other TS: 1,2-benzenedicarboxylic acid, Di-C8-C10 Branched Alkyl Esters, C9 Rich (CAS No. 68515-48-0)

**Method** : The calculated value was determined using MPBPWIN version 1.41, a subroutine within the computer program EPI Suite™ version 3.12. Melting Point estimations performed by MPBPWIN are based on the average result of the calculation methods of K. Joback and Gold and Ogle. Joback's Method is described in Joback, K.G. 1982. A Unified Approach to Physical Property Estimation Using Multivariate Statistical Techniques. In The Properties of Gases and Liquids. Fourth Edition. 1987. R.C. Reid, J.M. Prausnitz and B.E. Poling, Eds.  
The Gold and Ogle Method simply uses the formula  
 $T_m = 0.5839T_b$ , where  $T_m$  is the melting point in Kelvin and  $T_b$  is the boiling point in Kelvin.  
The SMILES notation used in the calculation was:

## 2. Physico-Chemical Data

Id 68515-48-0

Date 07.12.2006

**Remark** : O=C(c1ccccc1C(=O)O)O  
EPI Suite™ is used by the US EPA for estimating chemico-physical properties of substances. However, the melting point calculation in EPIWIN provides erroneously high results for phthalate esters.

**Test substance** : 1,2-benzenedicarboxylic acid, Di-C8-C10 Branched Alkyl Esters, C9 Rich (CAS No. 68515-48-0)

**Reliability** : (3) invalid  
06.06.2006 (6)

### 2.2 BOILING POINT

**Value** : = 454 °C at 1013 hPa  
**Decomposition** : no  
**Method** : other: calculated  
**Year** : 1999  
**GLP** :  
**Test substance** : other TS: 1,2-benzenedicarboxylic acid, Di-C8-C10 Branched Alkyl Esters, C9 Rich (CAS No. 68515-48-0)

**Method** : Boiling point calculated by MPBPWIN subroutine in EPI Suite™, which is based on the method of S. Stein and R. Brown in "Estimation of Normal Boiling Points from Group Contributions". 1994. J. Chem. Inf. Comput. Sci. 34: 581-587.  
The SMILES notation used in the calculation was:  
O=C(c1ccccc1C(=O)O)O

**Remark** : EPI Suite™ is used by the US EPA for estimating chemico-physical properties of substances.

**Test substance** : 1,2-benzenedicarboxylic acid, Di-C8-C10 Branched Alkyl Esters, C9 Rich (CAS No. 68515-48-0)

**Reliability** : (2) valid with restrictions  
The value was calculated based on chemical structure as modeled by EPI Suite™. This robust summary has a reliability rating of 2 because the data are calculated and not measured.

**Flag** : Critical study for SIDS endpoint  
06.06.2006 (6)

### 2.3 DENSITY

#### 2.3.1 GRANULOMETRY

### 2.4 VAPOUR PRESSURE

**Value** : = .0000000681 hPa at 25 °C  
**Decomposition** : no  
**Method** : other (calculated)  
**Year** :  
**GLP** :  
**Test substance** : other TS: 1,2-benzenedicarboxylic acid, Di-C8-C10 Branched Alkyl Esters, C9 Rich (CAS No. 68515-48-0)

**Remark** : Physicochemical data for selected commercial phthalate esters from various sources including the public literature, manufacturing specifications, and handbook values were evaluated by an industry peer review process. Valid values were identified and presented in a phthalate ester environmental fate, peer reviewed publication. These data including the

## 2. Physico-Chemical Data

Id 68515-48-0

Date 07.12.2006

values for vapor pressure represent the definitive and currently accepted physicochemical database for selected phthalate esters including diisononyl phthalate.

Quantitative structure-property relationships, significant at the 99.9% level, were developed using the relevant phthalate ester data to estimate solubility in water, air, and octanol, where V = the Le Bas molar volume (cm<sup>3</sup> mol<sup>-1</sup>). The Le Bas molar volume used for diisononyl phthalate ester was 564.8 cm<sup>3</sup> mol<sup>-1</sup>.

Log CS(WL) = -0.012V + 5.8, n = 35 (solubility in water)  
r<sup>2</sup> = 0.98, SE = 0.39

Log CS(AL) = -0.013V - 1.3, n = 15 (solubility in air)  
r<sup>2</sup> = 0.87, SE = 0.33

Log CS(OL) = -0.016V + 3.4, n = 68 (solubility in octanol)  
r<sup>2</sup> = 0.19, SE = 0.41

It was recommended by the authors that the above regressions be used for predicting the three solubilities for phthalate esters with alkyl chain lengths from 1 to 13 carbons.

**Test substance** : 1,2-benzenedicarboxylic acid, Di-C8-C10 Branched Alkyl Esters, C9 Rich (CAS No. 68515-48-0)

**Reliability** : (2) valid with restrictions

The value was calculated based on the QSPR (quantitative structure-property relationship) three-solubility model. This robust summary has a reliability rating of 2 because the data are calculated and not measured.

**Flag** : Critical study for SIDS endpoint  
06.06.2006

(3)

### 2.5 PARTITION COEFFICIENT

**Partition coefficient** : octanol-water

**Log pow** : = 8.6 at 25 °C

**pH value** :

**Method** : other (calculated)

**Year** :

**GLP** :

**Test substance** : other TS: 1,2-benzenedicarboxylic acid, Di-C8-C10 Branched Alkyl Esters, C9 Rich (CAS No. 68515-48-0)

**Remark** : Physicochemical data for 22 selected commercial phthalate esters from various sources including the public literature, manufacturing specifications, handbook values, and computer modeling were evaluated by an industry peer review process. Valid values were identified and presented in a phthalate ester physicochemical properties, peer reviewed publication. These data including the values for octanol-water partitioning represent the definitive and currently accepted physicochemical database for selected phthalate esters including diisononyl phthalate.

Quantitative structure-property relationships, significant at the 99.9% level, were developed using the relevant phthalate ester data to estimate solubility in water, air, and octanol, where V = the Le Bas molar volume (cm<sup>3</sup> mol<sup>-1</sup>). The Le Bas molar volume used for diisononyl phthalate ester was 564.8 cm<sup>3</sup> mol<sup>-1</sup>.

Log CS(WL) = -0.012V + 5.8, n = 35 (solubility in water)  
r<sup>2</sup> = 0.98, SE = 0.39

Log CS(AL) = -0.013V - 1.3, n = 15 (solubility in air)

## 2. Physico-Chemical Data

Id 68515-48-0

Date 07.12.2006

$r^2 = 0.87$ ,  $SE = 0.33$

$\text{Log CS(OL)} = -0.016V + 3.4$ ,  $n = 68$  (solubility in octanol)  
 $r^2 = 0.19$ ,  $SE = 0.41$

It was recommended by the authors that the above regressions be used for predicting the three solubilities for phthalate esters with alkyl chain lengths from 1 to 13 carbons.

**Test substance** : 1,2-benzenedicarboxylic acid, Di-C8-C10 Branched Alkyl Esters, C9 Rich (CAS No. 68515-48-0)

**Reliability** : (2) valid with restrictions

The value was calculated based on the QSPR (quantitative structure-property relationship) three-solubility model. This robust summary has a reliability rating of 2 because the data are calculated and not measured.

**Flag** : Critical study for SIDS endpoint  
06.06.2006

(3)

### 2.6.1 SOLUBILITY IN DIFFERENT MEDIA

**Solubility in** : Water  
**Value** : = .308 other: ug/l at 25 °C

**pH value** :  
**concentration** : at °C

**Temperature effects** :

**Examine different pol.** :  
**pKa** : at 25 °C

**Description** :

**Stable** :

**Deg. product** :

**Method** : other: calculated

**Year** :

**GLP** :

**Test substance** : other TS: 1,2-benzenedicarboxylic acid, Di-C8-C10 Branched Alkyl Esters, C9 Rich (CAS No. 68515-48-0)

**Remark** : Physicochemical data for 22 selected commercial phthalate esters from various sources including the public literature, manufacturing specifications, handbook values, and computer modeling were evaluated by an industry peer review process. Valid values were identified and presented in a phthalate ester physicochemical properties, peer reviewed publication. These data including the values for water solubility represent the definitive and currently accepted physicochemical database for selected phthalate esters including diisononyl phthalate.

Quantitative structure-property relationships, significant at the 99.9% level, were developed using the relevant phthalate ester data to estimate solubility in water, air, and octanol, where  $V$  = the Le Bas molar volume ( $\text{cm}^3 \text{mol}^{-1}$ ). The Le Bas molar volume used for diisononyl phthalate ester was  $564.8 \text{ cm}^3 \text{mol}^{-1}$ .

$\text{Log CS(WL)} = -0.012V + 5.8$ ,  $n = 35$  (solubility in water)  
 $r^2 = 0.98$ ,  $SE = 0.39$

$\text{Log CS(AL)} = -0.013V - 1.3$ ,  $n = 15$  (solubility in air)  
 $r^2 = 0.87$ ,  $SE = 0.33$

$\text{Log CS(OL)} = -0.016V + 3.4$ ,  $n = 68$  (solubility in octanol)  
 $r^2 = 0.19$ ,  $SE = 0.41$

It was recommended by the authors that the above regressions be used for



## 2. Physico-Chemical Data

Id 68515-48-0

Date 07.12.2006

predicting the three solubilities for phthalate esters with alkyl chain lengths from 1 to 13 carbons.

**Test substance** : 1,2-benzenedicarboxylic acid, Di-C8-C10 Branched Alkyl Esters, C9 Rich (CAS No. 68515-48-0)

**Reliability** : (2) valid with restrictions  
The value was calculated based on the QSPR (quantitative structure-property relationship) three-solubility model. This robust summary has a reliability rating of 2 because the data are calculated and not measured.

**Flag** : Critical study for SIDS endpoint  
06.06.2006 (3)

**Solubility in Value** :  
: = .61 other: ug/l at 21 °C

**pH value concentration** :  
: at °C

**Temperature effects** :  
: at 25 °C

**Examine different pol.** :  
: at 25 °C

**pKa** :  
: at 25 °C

**Description** :  
: Stable :  
: Deg. product :  
: Method : other: Slow Stir Procedure  
: Year :  
: GLP : yes

**Test substance** : other TS: 1,2-benzenedicarboxylic acid, Di-C8-C10 Branched Alkyl Esters, C9 Rich (CAS No. 68515-48-0)

**Remark** : A slow stir procedure was used. 100mg DINP was added to a closed carbon containing 12L of carbon-treated water that was then slowly stirred. The aqueous phase was sampled on days 1, 3, and 9 by extraction with a C18 extraction disk. Analysis was by gas chromatography with mass selective detection in the selective monitoring mode.

**Test substance** : 1,2-benzenedicarboxylic acid, Di-C8-C10 Branched Alkyl Esters, C9 Rich (CAS No. 68515-48-0)

06.06.2006 (10)

### 2.6.2 SURFACE TENSION

### 2.7 FLASH POINT

### 2.8 AUTO FLAMMABILITY

### 2.9 FLAMMABILITY

### 2.10 EXPLOSIVE PROPERTIES

### 2.11 OXIDIZING PROPERTIES

### 2.12 DISSOCIATION CONSTANT

## 2. Physico-Chemical Data

Id 68515-48-0  
Date 07.12.2006

### 2.13 VISCOSITY

### 2.14 ADDITIONAL REMARKS

### 3. Environmental Fate and Pathways

Id 68515-48-0

Date 07.12.2006

#### 3.1.1 PHOTODEGRADATION

Type : air  
Light source : Sun light  
Light spectrum : nm  
Relative intensity : 1 based on intensity of sunlight  
Conc. of substance : at 25 °C  
**INDIRECT PHOTOLYSIS**  
Sensitizer : OH  
Conc. of sensitizer : 1500000 molecule/cm<sup>3</sup>  
Rate constant : .000000000234 cm<sup>3</sup>/(molecule\*sec)  
Degradation : 50 % after 5.5 hour(s)  
Deg. product : not measured  
Method : other (calculated)  
Year :  
GLP :  
Test substance : other TS: 1,2-benzenedicarboxylic acid, Di-C8-C10 Branched Alkyl Esters, C9 Rich (CAS No. 68515-48-0)  
  
Method : Photodegradation rate calculated by AOPWIN ver. 1.91 based on the methods of Atkinson.  
Remark : 50% degradation after 5.48 hrs or 0.46 days based on a 12-hour day. The computer program AOPWIN (atmospheric oxidation program for Microsoft Windows) (EPI Suite<sup>TM</sup>, 2000) calculates a chemical half-life for a 12-hour day (the 12-hour day half-life value normalizes degradation to a standard day light period during which hydroxyl radicals needed for degradation are generated), based on an OH- reaction rate constant and a defined OH- concentration.  
EPI Suite<sup>TM</sup> is used and advocated by the US EPA for chemical property estimation.  
Test substance : 1,2-benzenedicarboxylic acid, Di-C8-C10 Branched Alkyl Esters, C9 Rich (CAS No. 68515-48-0)  
This robust summary has a reliability rating of 2 because the data are calculated.  
Flag : Critical study for SIDS endpoint  
06.07.2006 (6)

#### 3.1.2 STABILITY IN WATER

Type : abiotic  
t1/2 pH4 : at °C  
t1/2 pH7 : 7.7 year at 25 °C  
t1/2 pH9 : at °C  
Deg. product : not measured  
Method : other (calculated)  
Year :  
GLP :  
Test substance : other TS: 1,2-benzenedicarboxylic acid, Di-C8-C10 Branched Alkyl Esters, C9 Rich (CAS No. 68515-48-0)  
  
Method : Hydrolysis rate calculated by HYDROWIN ver. 1.67 based on work for EPA by T. Mill et al.  
Remark : EPI Suite<sup>TM</sup> is used and advocated by the US EPA for chemical property estimation.  
Test substance : 1,2-benzenedicarboxylic acid, Di-C8-C10 Branched Alkyl Esters, C9 Rich (CAS No. 68515-48-0)  
Reliability : (2) valid with restrictions

### 3. Environmental Fate and Pathways

Id 68515-48-0

Date 07.12.2006

**Flag**  
06.06.2006

This robust summary has a reliability rating of 2 because the data are calculated.  
: Critical study for SIDS endpoint

(6)

#### 3.1.3 STABILITY IN SOIL

#### 3.2.1 MONITORING DATA

#### 3.2.2 FIELD STUDIES

#### 3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

#### 3.3.2 DISTRIBUTION

**Media** : air - biota - sediment(s) - soil - water  
**Method** : Calculation according Mackay, Level I  
**Year** :

**Remark** : Physicochemical data used in the calculation:

Parameter	Value w/ Units
-----------	----------------

Molecular Weight	418.62
Temperature	25° C
Log Kow	8.6
Water Solubility	0.000308 g/m3
Vapor Pressure	0.00000681 Pa
Melting Point	-48°C

**Result** : Using the Mackay Level I calculation, the following distribution is predicted for diisononyl phthalate:

% Distribution	Compartment
0.0	Air
0.0	Water
97.7	Soil
2.2	Sediment
0.1	Suspended Sediment
0.0	Biota

**Test substance** : 1,2-benzenedicarboxylic acid, Di-C8-C10 Branched Alkyl Esters, C9 Rich (CAS No. 68515-48-0)

**Reliability** : (2) valid with restrictions  
This robust summary has a reliability rating of 2 because the data are calculated.

**Flag** : Critical study for SIDS endpoint  
06.06.2006

(16)

**Media** : air - biota - sediment(s) - soil - water  
**Method** : Calculation according Mackay, Level III  
**Year** :

**Remark** : Physicochemical data used in the calculation:

Parameter	Value w/ Units
-----------	----------------

### 3. Environmental Fate and Pathways

Id 68515-48-0

Date 07.12.2006

Molecular Weight 418.62  
Temperature 25° C  
Log Kow 8.6  
Water Solubility 0.000308 g/m3  
Vapor Pressure 0.00000681 Pa  
Melting Point -48°C  
Emissions rates used in the calculation:

Compartment Rate (kg/hr)

Air 1000  
Water 1000  
Soil 1000

Half-lives used in the calculation:

Compartment Half-life (hr)

Air 11.0a  
Water 120b  
Soil 420c  
Sediment 420c

a - as calculated using AOPWIN version 1.91, a subroutine of the computer program EPI Suite™ version 3.12 and normalized to a 24 hour day [Environmental Protection Agency (EPA) (2000). EPI Suite™, Estimation Program Interface Suite, v3.12. U.S. EPA, Washington, DC, USA.]

b - based on biodegradation data from: Exxon Biomedical Sciences, Inc. (1995) and Boethling (2000): Exxon Biomedical Sciences, Inc. (1995). Ready Biodegradability, Manometric Respirometry. Study No. 199894A. Unpublished report.

Boethling R (2000). HPVC-Screening Tool: Using Ready and Inherent Biodegradability Data to Derive Input Data for the EQC Model, Appendix 10 in Environment Canada, Environmental Categorization for Persistence Bioaccumulation and Inherent Toxicity of Substances on the Domestic Substance List Using QSARs, Results of an international workshop hosted by Chemicals Evaluation Division of Environment Canada, Nov. 11-12, 1999, in Philadelphia, PA, USA.

c - based on Boethling, R. recommendation that half-lives of 3 to 4 times longer than surface water should be used for soil and sediment.

#### Result

: Using the Mackay Level III calculation, the following distribution is predicted for diisononyl phthalate:

Compartment % Distribution  
Air 0.9  
Water 8.2  
Soil 68.5  
Sediment 22.4

#### Test substance

: 1,2-benzenedicarboxylic acid, Di-C8-C10 Branched Alkyl Esters, C9 Rich (CAS No. 68515-48-0)

#### Reliability

: (2) valid with restrictions  
This robust summary has a reliability rating of 2 because the data are calculated.

#### Flag

06.06.2006

: Critical study for SIDS endpoint

(16)

#### 3.4 MODE OF DEGRADATION IN ACTUAL USE

#### 3.5 BIODEGRADATION

**Type** : aerobic  
**Inoculum** : activated sludge, domestic, non-adapted  
**Contact time** : 28 day(s)  
**Degradation** : = 70.5 (±) % after 28 day(s)  
**Result** : readily biodegradable  
**Deg. product** :  
**Method** : OECD Guide-line 301 F "Ready Biodegradability: Manometric Respirometry Test"  
**Year** : 1994  
**GLP** : no  
**Test substance** : other TS: 1,2-benzenedicarboxylic acid, Di-C8-C10 Branched Alkyl Esters, C9 Rich (CAS No. 68515-48-0)

**Result** : The biodegradation half-life <3 weeks. By day 28, 70.5% degradation of the test substance was observed. 10% biodegradation was achieved on approximately day 12, 50% biodegradation on approximately day 18, and >60% biodegradation on day 22.

By day 14, >60% biodegradation of positive control was observed, which meets the guideline requirement. Oxygen uptake of the blanks were within guideline limits. No excursions from the protocol were noted.

Biodegradation was based on oxygen consumption and the theoretical oxygen demand of the test substance as calculated using results of an elemental analysis of the test substance.

##### Test Substance:

Day	% Degradation*
10	2, 3, 2
11	5, 10, 8
12	13, 18, 13
17	51, 51, 36
22	68, 66, 50
28	79, 74, 58 (mean = 70.5)

##### Positive Reference Substance (Na Benzoate):

Day	% Degradation*
1	32, 36, 34
2	56, 66, 61
5	76, 89, 82

\* replicate data

**Test condition** : Activated sludge and test medium were combined prior to test substance addition. Test medium consisted of glass distilled water and mineral salts (phosphate buffer, ferric chloride, magnesium sulfate, calcium chloride).

Test vessels were 1L glass flasks placed in a waterbath and electronically monitored for oxygen consumption. Test substance was tested in triplicate, controls and blanks were tested in duplicate.

Test substance (1,2-benzenedicarboxylic acid, diiso-C9 alkyl esters) concentration was approximately 50 mg/L. The positive control (sodium benzoate) concentration was approximately 50 mg/L. Test temperature was 22 +/- 1 Deg C.

### 3. Environmental Fate and Pathways

Id 68515-48-0

Date 07.12.2006

	All test vessels were stirred constantly for 28 days using magnetic stir bars and plates.
<b>Test substance</b>	: 1,2-benzenedicarboxylic acid, Di-C8-C10 Branched Alkyl Esters, C9 Rich (CAS No. 68515-48-0). No information on purity, but believed to represent 100% commercial product.
<b>Conclusion</b>	: The test substance is readily biodegradable.
<b>Reliability</b>	: (1) valid without restriction This summary is rated a "1" and represents a key study because it followed an OECD standard guideline, which describes a procedure specifically designed to evaluate this endpoint, and the results were reviewed for reliability and assessed as valid.
<b>Flag</b> 07.12.2006	: Critical study for SIDS endpoint (7)
<b>Type</b>	: aerobic
<b>Inoculum</b>	: activated sludge, domestic, adapted
<b>Concentration</b>	: 20 mg/l related to Test substance related to
<b>Contact time</b>	: 28 day(s)
<b>Degradation</b>	: = 62 (±) % after 28 day(s)
<b>Result</b>	:
<b>Deg. product</b>	:
<b>Method</b>	: other: USEPA 1982, CO2 Evolution, Shake Flask
<b>Year</b>	: 1983
<b>GLP</b>	: yes
<b>Test substance</b>	: other TS: 1,2-benzenedicarboxylic acid, Di-C8-C10 Branched Alkyl Esters, C9 Rich (CAS No. 68515-48-0)
<b>Method</b>	: Inoculum - Acclimated domestic sewage and soil Kinetics - Not reported Degradation Products - Not reported Analytical Monitoring - Yes
<b>Result</b>	: Primary degradation was expressed as the loss of test substance as determined by chemical analysis. Ultimate biodegradation was expressed as percentage CO2 evolved based on total theoretical CO2. >99% primary degradation 62% (sd 2.0) ultimate biodegradation
<b>Test condition</b>	: The inoculum was acclimated for 2 weeks prior to test initiation. The test substance was added to flasks that contained medium and inoculum. The flasks were incubated and shaken in the dark for 28 days. Three replicates for CO2 evolution and 4 replicates for primary degradation were evaluated. CO2 produced was captured in barium hydroxide solution and measured by titration. Primary biodegradation was determined at the beginning, middle, and end of the test period by GC-FID (gas chromatographic flame ionization detection) analysis of the entire contents of one replicate. Glucose (positive control) and blank (control) test systems were also evaluated. The test results were corrected for CO2 produced in the blank test systems. 2L Erlenmeyer flasks were used as test vessels. The pH at initiation was 7.0 to 7.2. Test flasks were shaken at a rate of 120 rpm at 22 +/- 2 Deg C. Nominal test concentration = 20 mg/L for test substance and glucose.
<b>Test substance</b>	: 1,2-benzenedicarboxylic acid, Di-C8-C10 Branched Alkyl Esters, C9 Rich (CAS No. 68515-48-0) Synonym: DINP
<b>Conclusion</b>	: The data developed in this study which used an acclimated inoculum and the remaining biodegradation data summarized by Staples et al. (1997b), which include both acclimated and unacclimated data, clearly show that high molecular weight phthalate esters, including diisononyl phthalate ester, biodegrade rapidly and to a great extent.
<b>Reliability</b>	: (1) valid without restriction This summary is rated a "1" and represents a key study because it followed a USEPA standard guideline, which describes a procedure specifically

### 3. Environmental Fate and Pathways

Id 68515-48-0  
Date 07.12.2006

designed to evaluate this endpoint, and the results were reviewed for reliability and assessed as valid.

07.12.2006

(23) (25)

**3.6 BOD5, COD OR BOD5/COD RATIO**

**3.7 BIOACCUMULATION**

**3.8 ADDITIONAL REMARKS**



## 4.1 ACUTE/PROLONGED TOXICITY TO FISH

**Type** : flow through  
**Species** : Oncorhynchus mykiss (Fish, fresh water)  
**Exposure period** : 96 hour(s)  
**Unit** : mg/l  
**LC50** : > .16  
**Limit test** :  
**Analytical monitoring** : yes  
**Method** : other  
**Year** : 1975  
**GLP** : yes  
**Test substance** : other TS: 1,2-benzenedicarboxylic acid, Di-C8-C10 Branched Alkyl Esters, C9 Rich (CAS No. 68515-48-0)

**Method** : Method/Guideline-USEPA, (660/3-75-009) Methods for Acute Toxicity Tests with Fish, 1975. Macroinvertebrates, and Amphibians.

Statistical methods-Moving average angle, Probit or Bionomial concentration.

**Result** : 96 hr LC50 >0.16 mg/L  
 Mean measured values were used in the LC50 calculation.

Nominal test concentrations: control, 0.012, 0.025, 0.050, 0.10, and 0.20 ul/L.

Mean measured test concentrations: < 0.0068 (control), 0.0087, 0.019, 0.032, 0.062, and 0.16 mg/L.

Analytical samples were taken at time zero and on a composite of replicates at study termination. Measured values dropped slightly during the exposure period.

% Mortality results at 96 hrs per replicate for control and treatment levels:  
 Conc. (mg/L)    Rep1/Rep2

Control	0 / 0
0.0087	0 / 0
0.019	0 / 0
0.032	0 / 0
0.062	0 / 0
0.16	0 / 0

**Test condition** : Test treatments were prepared by using a proportional diluter modified to enhance mixing of phthalates. The dilution water was Wareham Mass. town water (untreated and unchlorinated). A concentrated stock solution was prepared and combined with dilution water prior to pumping into the diluter. The diluter delivered a series of stock dilutions to the test vessels. Test chambers were glass tanks containing 15 L of solution. The diluter maintained a water turnover rate of 5 to 8 tank volumes per day. Two replicates of ten organisms were tested per treatment and control. Analytical method was Gas Liquid Chromatography (GLC) with electron capture detection.

Fish mean length = 39 mm and mean wet weight = 0.5 g. Test temperature = 11 Deg C. The pH ranged from 7.1 to 7.4. The mean dissolved oxygen ranged from 10.0 to 10.1 mg/L. Ranges of total hardness and alkalinity as CaCO<sub>3</sub> of the dilution water were 20 to 26 mg/L and 14 to 22 mg/L, respectively.

Fish were obtained from a Montana supplier.

<b>Test substance</b>	: 1,2-benzenedicarboxylic acid, Di-C8-C10 Branched Alkyl Esters, C9 Rich (CAS No. 68515-48-0). Purity: 100% active ingredient.
<b>Conclusion</b>	: Test substance is non-toxic to fish at or below its water solubility level. Data selected based upon routine species, measured data and representative value, as compared with those found in reference document, Staples et al. (1997).
<b>Reliability</b>	: (1) valid without restriction This summary is rated a "1" and represents a key study because it followed an U.S. EPA standard guideline, which describes a procedure specifically designed to evaluate this endpoint, and the results were reviewed for reliability and assessed as valid.
<b>Flag</b> 07.12.2006	: Critical study for SIDS endpoint (5) (24)

#### 4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

<b>Type</b>	: static
<b>Species</b>	: Daphnia magna (Crustacea)
<b>Exposure period</b>	: 48 hour(s)
<b>Unit</b>	: mg/l
<b>LC50</b>	: > .06
<b>Analytical monitoring</b>	: yes
<b>Method</b>	: other
<b>Year</b>	: 1975
<b>GLP</b>	: yes
<b>Test substance</b>	: other TS: 1,2-benzenedicarboxylic acid, Di-C8-C10 Branched Alkyl Esters, C9 Rich (CAS No. 68515-48-0)
<b>Method</b>	: Method/Guideline-USEPA, (660/3-75-009) Methods for Acute Toxicity Tests with Fish, Macroinvertebrates, and Amphibians. 1975. Statistical methods incorporated the following procedures: Moving average angle, Probit, and Binomial Probability.
<b>Result</b>	: 48 hr EC50 >0.086 mg/L (based upon time zero analytical samples; no effects at test substance saturation). Value was recalculated as >0.06 mg/L as per U.S. EPA current practices using mean of measured initiation and termination samples as reported in Staples et al. (1997).  Mean measured values were used in the final EC50 calculation. This study was conducted as a limit test.  Nominal test concentrations: control and 0.20 mg/L. Mean measured test concentrations of time 0 and 48 hr values: <0.014 and 0.06 mg/L.  Analytical samples taken at time zero and on a composite of replicates at termination. Measured values declined to a level at or below the detection limit during study exposure. The high treatment solution is considered the maximum solubility achievable under the conditions of the test.  % Immobility results at 48 hrs per replicate for control and treatment level: Conc. (mg/L)    Rep1/Rep2/Rep3  Control            0 / 0 / 0 0.06              0 / 0 / 0
<b>Test condition</b>	: The test treatment was prepared by mixing the test substance and dilution water (fortified well water) using a magnetic stir bar at a loading of 10 ul per liter. Exposure solution was removed from below the surface of the mixing vessel after settling for 1 hour and transferred to a Mariotte bottle and allowed to settle again for 24 hours, after which solution from below the surface was removed for use in the test. Three replicates of five organisms

## 4. Ecotoxicity

Id 68515-48-0

Date 07.12.2006

were tested at a single treatment level. Test vessels were 250 ml beakers with 200 ml of test solution. Analytical method was Gas Liquid Chromatography (GLC).  
Test temperature = 22 +/- 2 Deg C. The pH was 8.4 at test initiation and 8.4 on Day 2. Dissolved Oxygen ranged from 8.6 to 9.7 at test initiation and was 8.3 on Day 2. The range of total hardness of the dilution water was 150 to 170 mg/L. Daphnia were <24 hours old and obtained from in-house stock.

**Test substance** : 1,2-benzenedicarboxylic acid, Di-C8-C10 Branched Alkyl Esters, C9 Rich (CAS No. 68515-48-0)  
Synonym: DINP  
Purity: unstated, but believed to be 100% active ingredient because the test material came from the same source as in the rainbow trout acute study.

**Conclusion** : Test substance is non-toxic to Daphnia at or below its water solubility level. Data selected based upon routine species, measured data and representative value, as compared with those found in reference document, Staples et al. (1997).

**Reliability** : (1) valid without restriction  
This summary is rated a "1" and represents a key study because it followed an U.S. EPA standard guideline, which describes a procedure specifically designed to evaluate this endpoint, and the results were reviewed for reliability and assessed as valid.

**Flag** : Critical study for SIDS endpoint  
07.12.2006 (20) (24)

### 4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

**Species** : Selenastrum capricornutum (Algae)  
**Endpoint** : other: chlorophyll a  
**Exposure period** : 5 day(s)  
**Unit** : mg/l  
**NOEC** : = 1.8  
**EC50** : > 1.8  
**Limit test** :  
**Analytical monitoring** : yes  
**Method** : other  
**Year** : 1978  
**GLP** : yes  
**Test substance** : other TS: 1,2-benzenedicarboxylic acid, Di-C8-C10 Branched Alkyl Esters, C9 Rich (CAS No. 68515-48-0)

**Method** : Method/Guideline - EPA 600/9-78-018, Printz Algal Assay Bottle Test. 1978.  
Statistical methods - Moving average angle, Probit or Bionomial  
Test type - Static

**Result** : 120 hr (5 day) EC50 >2.8 mg/L (based upon time zero analytical samples). Value was recalculated as >1.8 mg/L as per U.S. EPA current practices using mean of measured initiation and termination samples as reported in Staples et al. (1997).

Mean measured values were used in the final EC50 calculation.

Nominal test concentration as a percent of a saturated solution: 0 (control) and 100.0%.

Mean measured test concentrations of time 0 and 120 hr values: <0.10 and 1.8 mg/L (detection limit was 0.10 mg/L).

Analytical samples taken at time zero and on a composite of replicates at termination. In-vivo chlorophyll a, measured until less than 5% change.

Both cell number and in-vivo chlorophyll a, measured at termination. Control chlorophyll a or cell counts were not reported. Analytical samples were taken at time zero and on a composite of replicates at termination.

Chlorophyll a percent change relative to control on sampling days and cell number on day 6 results:

Conc. Chlorophyll a percent change from control  
(mg/L) Day 1 Day 2 Day 3 Day 4 Day 5 Cell # Day 5  
1.8 -6 -10 -72 -16 -12 -34

**Test condition**

- : Algal Growth Medium was used as the control and diluent. 10 uL of test substance was added to 1.0 L of sterile water to form a saturated phthalate solution. This solution was sonicated for 1 minute and allowed to settle for 4 hours. After settling, the water soluble fraction (WSF) was removed for testing. Initial algal concentration was 2.0 E4 cells/ml. Only one treatment level was evaluated (100% WSF) because earlier phthalate testing suggested that toxic effects were not expected with higher molecular weight phthalate esters with low water solubility.

**Test substance**

- : Lighting = 4,700 lux, Test temperature = 22+/-2 Deg C. The pH was 7.4 at initiation and was not measured on day 5. Algal culture stock was obtained from University of Texas at Austin, TX.  
: 1,2-benzenedicarboxylic acid, Di-C8-C10 Branched Alkyl Esters, C9 Rich (CAS No. 68515-48-0)  
Synonym: DINP  
Purity: unstated, but believed to be 100% active ingredient as was provided in the rainbow trout study.

**Conclusion**

- : Test substance is not toxic to algae at or below its water solubility level. Data selected based upon routine species, measured data and representative value, as compared with those found in reference document, Staples et al (1997).

Test substance is not toxic to algae at or below the solubility level in test medium used in this study.

**Reliability**

- : The alga (*Selenastrum capricornutum*) toxicity data reported for diisononyl phthalate ester are consistent with the data for several high molecular weight phthalate esters as summarized by Staples et al. (1997). These data clearly showed that high molecular weight phthalate esters, including diisononyl phthalate ester, do not produce toxicity to *S. capricornutum* at or below their maximum attainable solubility.  
: (1) valid without restriction  
The study procedure followed an accepted test guideline and applied GLP. The data are consistent with known toxicological properties of similar high molecular weight phthalate ester substances. Control chlorophyll or cell counts not reported.

07.12.2006

(21) (24)

**4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA****4.5.1 CHRONIC TOXICITY TO FISH**

**Species** : *Oryzias latipes* (Fish, fresh water)  
**Endpoint** :  
**Exposure period** : 284 day(s)  
**Unit** :  
**Analytical monitoring** : yes  
**Method** :  
**Year** : 2001

## 4. Ecotoxicity

Id 68515-48-0

Date 07.12.2006

**GLP** :  
**Test substance** : other TS: 1,2-benzenedicarboxylic acid, Di-C8-C10 Branched Alkyl Esters, C9 Rich (CAS No. 68515-48-0)

**Remark** : Test substance was tested in a multi-generation dietary exposure protocol to evaluate reproductive and developmental effects in the Japanese Medaka. Test substance was spiked via an acetone solution into a fish flake food at 20µg/g. Fish were fed at a daily rate of 5% body weight / day. Fo and F1 generation adults were reared through sexual maturation and ovipositor (140 days-post-hatch). Test ended with F2 generation prior to sexual maturation.

Effects were evaluated using population, individual, and biochemical parameters including: survival, sex ratio, fecundity, development, growth, gonadal-somatic index, histopathology, testosterone metabolism, EROD activity, and vitellogenin production.

Results indicated that egg production was similar among all treatment groups. F1 and F2 generation embryos showed normal development except for transient change in red blood cell pigmentation in the phthalate and acetone groups. There were no treatment-related alterations in survival, fecundity, or GSI and no histological lesions were observed.

There was no shift in male-to-female ratio and the phenotypic and histological gender classifications for both male and female fish were in agreement. Testosterone metabolism, EROD activity, and vitellogenin levels were not significantly different among treatment groups.

**Test substance** : 1,2-benzenedicarboxylic acid, Di-C8-C10 Branched Alkyl Esters, C9 Rich (CAS No. 68515-48-0)

**Reliability** : (1) valid without restriction  
07.12.2006

(18)

### 4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

**Species** : Daphnia magna (Crustacea)  
**Endpoint** : reproduction rate  
**Exposure period** : 21 day(s)  
**Unit** : mg/l  
**NOEC** : = 1.05  
**EC50** : > 1.05  
**Analytical monitoring** : yes  
**Method** : OECD Guide-line 202, part 2 "Daphnia sp., Reproduction Test"  
**Year** : 1984  
**GLP** : yes  
**Test substance** : other TS: 1,2-benzenedicarboxylic acid, Di-C8-C10 Branched Alkyl Esters, C9 Rich (CAS No. 68515-48-0)

**Method** : The test method followed the Daphnid chronic testing procedure described in OECD guideline 202 (1984) with the use of a dispersant, castor oil 40-ethoxylate (Marlowet 40), in accordance with guideline specifications.

**Result** : Daphnia parent (Po) survival, reproduction (cumulative number of offspring, F1, per live parent), and parent length were evaluated as the biological endpoints. Diisononyl phthalate ester showed no effect on survival, reproduction, and length at a loading of 1.0 mg/L test substance and 10 mg/L dispersant under the conditions of this test.

	Control	Dispersant	Control	Test Substance
Po % Mortality	0	10		10
Mean F1/ Surviving Po	93 (sd=9)	106 (sd=10)		100 (sd=12)

<b>Test condition</b>	<p>Po Mean Length 4.1 (sd=0.17) 4.1 (sd=0.17) 4.2 (sd=0.18)</p> <p>: Test substance exposure solutions were prepared using stock dispersions prepared by adding 100 mg substance and 1000 mg dispersant (castor oil 40-ethoxylate; Marlowet 40), then bringing the test solution to 1 L by adding dilution medium. The dilution medium was Elendt's medium (Elendt and Bias, 1990), which was pH adjusted to 8 and aerated for &gt;2 hours prior to use.</p> <p>Ten replicate test systems with 1 daphnid each (&lt; 24 hours old) were prepared in glass beakers with loose fitting lids. Each beaker contained 80 ml of exposure solution with a depth of approximately 5 cm. The photoperiod was controlled to 16 hours light and 8 hours dark with a 15 minute transition period.</p> <p>The exposure solution was renewed every Monday, Wednesday, and Friday. On each renewal day the parent organism (Po) was transferred to a new exposure solution and neonates (F1) were counted. Water quality measurements including dissolved oxygen concentration and pH were determined at every renewal for the new and old exposure and control solutions. Test conditions were:</p> <p style="padding-left: 40px;">Temperature = 20 +/- 1.0 degree C  Water hardness = &gt;140 mg/L (as CaCO<sub>3</sub>)  Alkalinity = &gt;100 mg/L (as CaCO<sub>3</sub>)  pH = approximately 8  Dissolved oxygen = 8-9 mg/L</p> <p>Standard daily feeding rates with the cultured alga, <i>Chlorella vulgaris</i>, was supplemented with microencapsulated food, "Frippak Booster".</p> <p>Test substance analyses of new and old exposure solutions were performed using gas chromatography with flame ionization detection, after a hexane extraction. The mean measured test substance concentrations were 1.1 mg/L in new exposure solutions and 1.0 mg/L in old exposure solutions, which represents 110 and 100%, respectively, of the nominally added test substance.</p>
<b>Test substance</b>	: 1,2-benzenedicarboxylic acid, Di-C8-C10 Branched Alkyl Esters, C9 Rich (CAS No. 68515-48-0); purity >99.5%
<b>Conclusion</b>	: Chronic invertebrate ( <i>Daphnia magna</i> ) toxicity data reported for diisononyl phthalate ester are consistent with valid data for several high molecular weight phthalate esters as summarized by Brown et al. (1998), Staples et al. (1997), and Rhodes et al. (1995). These data show that high molecular weight phthalate esters, including diisononyl phthalate ester, do not produce chronic toxicity to <i>Daphnia magna</i> . Testing was conducted at a loading that exceeds the water solubility of diisononyl phthalate ester (0.61 ug/L; Letinski et al., 2002) after it was demonstrated that such a procedure was able to satisfactorily disperse the test substance and that it prevented floatation of the test organism, a documented problem that can occur when evaluating the toxicity of similar substances.
<b>Reliability</b>	: (1) valid without restriction The study procedure followed an accepted test guideline and applied GLP. The study procedure and results were accepted in a peer reviewed journal. The data are consistent with known toxicological properties of similar high molecular weight phthalate ester substances.
<b>Flag</b> 07.12.2006	: Critical study for SIDS endpoint (2) (15) (19) (24)
<b>Species</b>	: <i>Daphnia magna</i> (Crustacea)
<b>Endpoint</b>	: other: survival and reproduction
<b>Exposure period</b>	: 21 day(s)
<b>Unit</b>	: mg/l
<b>NOEC</b>	: = .034
<b>Analytical monitoring</b>	: yes

## 4. Ecotoxicity

Id 68515-48-0

Date 07.12.2006

**Method** : other: EG&G Bionomics chronic toxicity test  
**Year** : 1982  
**GLP** : yes  
**Test substance** : other TS: 1,2-benzenedicarboxylic acid, Di-C8-C10 Branched Alkyl Esters, C9 Rich (CAS No. 68515-48-0)

**Remark** : The study was confounded by surface filming and surface entrapment of test organisms. The results after 21 days showed effects on survival and reproduction in comparison to the controls for the two high concentrations. However, these effects are attributed to physical effects associated with testing this hydrophobic liquid at concentrations well in excess of water solubility. Consequently, the results of this study are concluded not to be valid for toxicity assessment.

**Test substance** : 1,2-benzenedicarboxylic acid, Di-C8-C10 Branched Alkyl Esters, C9 Rich (CAS No. 68515-48-0)

**Reliability** : (3) invalid  
07.12.2006

(22)

### 4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

### 4.6.2 TOXICITY TO TERRESTRIAL PLANTS

### 4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

### 4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

### 4.7 BIOLOGICAL EFFECTS MONITORING

### 4.8 BIOTRANSFORMATION AND KINETICS

### 4.9 ADDITIONAL REMARKS

## 5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

## 5.1.1 ACUTE ORAL TOXICITY

Type : LD50  
Value : > 10000 mg/kg bw  
Species : rat  
Strain : Sprague-Dawley  
Sex : male  
Number of animals : 30  
Vehicle : no data  
Doses :  
Method : other: not specified  
Year :  
GLP : no data  
Test substance : other TS: 1,2-benzenedicarboxylic acid, Di-C8-C10 Branched Alkyl Esters, C9 Rich (CAS No. 68515-48-0)

Remark : DINP was administered by gastric intubation to groups of 5 fasted rats. Dose levels: 34.6, 120, 417, 1450, 5000 and 10,000 mg/kg of body weight. A 14 day observation was used. No deaths occurred at any of the levels tested. Depressed, laboured respiration and oily-appearing fur were noted at levels of 5000 mg/kg and above. Recovery occurred within three to seven days. Weight loss was observed at 10,000 mg/kg. No major necropsy findings were observed at any dose level.

Test substance : 1,2-benzenedicarboxylic acid, Di-C8-C10 Branched Alkyl Esters, C9 Rich (CAS No. 68515-48-0)

Conclusion : The acute oral LD50 is greater than 10,000 mg/kg/day.  
07.12.2006 (14)

## 5.1.2 ACUTE INHALATION TOXICITY

## 5.1.3 ACUTE DERMAL TOXICITY

Type : LD50  
Value : > 3160 mg/kg bw  
Species : rabbit  
Strain :  
Sex :  
Number of animals : 16  
Vehicle : no data  
Doses :  
Method : other: not specified  
Year :  
GLP : no data  
Test substance : other TS: 1,2-benzenedicarboxylic acid, Di-C8-C10 Branched Alkyl Esters, C9 Rich (CAS No. 68515-48-0)

Remark : A single 24-hour application of DINP was applied at concentrations of 50, 200, 794 and 3160 mg/kg to the abraded rabbit skin under occlusive covering (n = 4). A 14 day observation period was used. There were no deaths and no evidence of systemic toxicity at any dose level.

Test substance : 1,2-benzenedicarboxylic acid, Di-C8-C10 Branched Alkyl Esters, C9 Rich



**Conclusion** : (CAS No. 68515-48-0)  
07.12.2006 : The acute dermal LD50 is greater than 3160 mg/kg. (13)

### 5.1.4 ACUTE TOXICITY, OTHER ROUTES

### 5.2.1 SKIN IRRITATION

### 5.2.2 EYE IRRITATION

### 5.3 SENSITIZATION

### 5.4 REPEATED DOSE TOXICITY

### 5.5 GENETIC TOXICITY 'IN VITRO'

**Type** : Ames test  
**System of testing** : Salmonella strains TA98, 100, 1535, 1537 and 1538  
**Test concentration** : 0.5 to 5000 ug/plate  
**Cycotoxic concentr.** :  
**Metabolic activation** : with and without  
**Result** : negative  
**Method** : OECD Guide-line 471  
**Year** : 1983  
**GLP** : yes  
**Test substance** : other TS: 1,2-benzenedicarboxylic acid, Di-C8-C10 Branched Alkyl Esters, C9 Rich (CAS No. 68515-48-0)

**Test substance** : 1,2-benzenedicarboxylic acid, Di-C8-C10 Branched Alkyl Esters, C9 Rich (CAS No. 68515-48-0)  
07.12.2006 (9) (17)

**Type** : Cytogenetic assay  
**System of testing** : Chinese hamster ovary cells  
**Test concentration** : 5 to 160 ug/ml  
**Cycotoxic concentr.** :  
**Metabolic activation** : with and without  
**Result** : negative  
**Method** : OECD Guide-line 473  
**Year** : 1983  
**GLP** : yes  
**Test substance** : other TS: 1,2-benzenedicarboxylic acid, Di-C8-C10 Branched Alkyl Esters, C9 Rich (CAS No. 68515-48-0)

**Test substance** : 1,2-benzenedicarboxylic acid, Di-C8-C10 Branched Alkyl Esters, C9 Rich (CAS No. 68515-48-0)  
07.12.2006 (8) (17)

**Type** : Mouse lymphoma assay  
**System of testing** : forward mutation assay, cell line L5178Y  
**Test concentration** : 500 - 8000 nl/ml  
**Cycotoxic concentr.** :

## 5. Toxicity

Id 68515-48-0

Date 07.12.2006

**Metabolic activation** : with and without  
**Result** : negative  
**Method** : other: Clive and Spector. Mutat. Res. 31:17-29.  
**Year** : 1975  
**GLP** : yes  
**Test substance** : other TS: mixture of commercial DINPs

06.06.2006

(1)(12)

**Type** : Mouse lymphoma assay  
**System of testing** : forward mutation assay, cell line L5178Y  
**Test concentration** : 7.5 - 100 ul/ml  
**Cytotoxic concentr.** :  
**Metabolic activation** : with and without  
**Result** : negative  
**Method** : other: modification of Clive and Spector. Mutat. Res. 31:17-29.  
**Year** : 1975  
**GLP** : yes  
**Test substance** : other TS: mixture of commercial DINPs

22.06.2006

(4)

### 5.6 GENETIC TOXICITY 'IN VIVO'

**Type** : Micronucleus assay  
**Species** : mouse  
**Sex** : male/female  
**Strain** : CD-1  
**Route of admin.** : gavage  
**Exposure period** : one exposure  
**Doses** : 500, 1000, 2000  
**Result** : negative  
**Method** : other  
**Year** : 2000  
**GLP** : yes  
**Test substance** : other TS: 1,2-benzenedicarboxylic acid, Di-C8-C10 Branched Alkyl Esters, C9 Rich (CAS No. 68515-48-0)

**Method** : Schmid W. The micronucleus test. Mutat. Res. 1975; 31: 9-15.

In vivo mammalian bone marrow micronucleus, oral gavage. Performed by Exxon Biomedical Sciences, Inc. (2000). Final Report.

**Test substance** : 1,2-benzenedicarboxylic acid, Di-C8-C10 Branched Alkyl Esters, C9 Rich (CAS No. 68515-48-0)

**Conclusion** : DINP was inactive in an in vivo micronucleus test that utilized a multiple-treatment, single-sacrifice study design. Because an initial range-finding test had shown that there were no differences between males and females, the definitive test utilized male mice only. Frequency of micronucleus formation was not elevated at any dose and there was no evidence of toxicity.

07.12.2006

(17)

### 5.7 CARCINOGENICITY

#### 5.8.1 TOXICITY TO FERTILITY

**Type** : Two generation study

## 5. Toxicity

Id 68515-48-0

Date 07.12.2006

**Species** : rat  
**Sex** : male/female  
**Strain** : Fischer 344  
**Route of admin.** : oral feed  
**Exposure period** : up to 26 weeks  
**Frequency of treatm.** : daily  
**Premating exposure period**  
    **Male** : ten weeks (6 weeks old)  
    **Female** : ten weeks (6 weeks old)  
**Duration of test** : up to 26 weeks  
**No. of generation studies** :  
**Doses** : 0.2%, 0.4%, 0.8% (n=30/sex/group)  
**Control group** : yes, concurrent no treatment  
**NOAEL parental** : .8 %  
**NOAEL F1 offspring** : .8 %  
**NOAEL F2 offspring** : .8 %  
**Method** : other: Directive 67/548/EEC, Part B and OECD Guideline 414  
**Year** :  
**GLP** : yes  
**Test substance** : other TS: 1,2-benzenedicarboxylic acid, Di-C8-C10 Branched Alkyl Esters, C9 Rich (CAS No. 68515-48-0)

**Remark** : The potential reproductive toxicity of di-isononyl phthalate was assessed in one and two-generation reproductive toxicity studies. Groups of 30 male and female CRL:CD(SD)BR rats were given DINP via dietary administration at levels of either 0.0, 0.5, 1, or 1.5% (one generation study) or 0.0, 0.2, 0.4, or 0.8% (two generation study).

There were no changes in any of the classic reproductive parameters, i.e., mating, male or female fertility, fecundity, gestational index, or length of gestation in either study. The overall NOAELs for these effects were the highest dietary levels (%) tested ~ 500 mg/kg/day in the two generation study and 1000 mg/kg/day in the one-generation study. Adult survival was unaffected at any level in either study.

### Two-generation study:

In the two-generation study there were no testicular effects in either the P1 males, exposed as juveniles and young adults or the P2(F1) offspring exposed in utero, through lactation, and continuously to terminal sacrifice. The NOAEL was 470 mg/kg/day.

### One-generation study:

Offspring survival was reduced at the 1.5% level (~ 1100 mg/kg/day) but unaffected at the 1% level (~ 760 mg/kg/day). Offspring body weights were decreased both at postnatal day (PND 0) and during lactation; however, the PND 0 effects were only clearly related to treatment at the 1.5% level. Weights of offspring during lactation were significantly reduced but within the historical control range at dietary levels (%) below 1%. As there was rapid recovery at the lower levels, even though treatment continued, the toxicologic significance is unclear. Weight gain was significantly reduced at the 1% level (~ 600 mg/kg/day). Liver and kidney weights were elevated at dietary level (%) above ~ 110 mg/kg/day, consistent with evidence from other studies of peroxisomal proliferation at these levels.

**Test substance** : 1,2-benzenedicarboxylic acid, Di-C8-C10 Branched Alkyl Esters, C9 Rich (CAS No. 68515-48-0)

**Conclusion** : This study showed that DINP treatment did not affect fertility or male reproductive development at doses of up to approximately 1000 mg/kg/day.  
07.12.2006 (11) (27)

## 5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

Species	: rat
Sex	: female
Strain	: other: Crl:CDBR
Route of admin.	: gavage
Exposure period	: Gestation Days 6-15
Frequency of treatm.	: daily
Duration of test	: 21 days
Doses	: 0, 100, 500, and 1000 mg/kg/day
Control group	: yes
NOAEL maternal tox.	: = 500 mg/kg bw
NOAEL teratogen.	: = 500 - mg/kg bw
Method	: Directive 87/302/EEC, part B, p. 24 "Teratogenicity test - rodent and non-rodent"
Year	:
GLP	: yes
Test substance	: other TS: 1,2-benzenedicarboxylic acid, Di-C8-C10 Branched Alkyl Esters, C9 Rich (CAS No. 68515-48-0)
Result	: DINP was not a selective developmental toxicant, nor was it embryotoxic or teratogenic under conditions of this study.
Test substance	: 1,2-benzenedicarboxylic acid, Di-C8-C10 Branched Alkyl Esters, C9 Rich (CAS No. 68515-48-0)
Conclusion	: The highest level (1000 mg/kg/day) reduced maternal weight gain and increased the incidence of developmental variations. The middose (500 mg/kg/day) was a NOAEL for both maternal and fetal effects.

07.12.2006

(26)

## 5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

Type	: other: Two generation study
In vitro/in vivo	:
Species	: rat
Sex	: male/female
Strain	: Fischer 344
Route of admin.	: oral feed
Exposure period	: up to 26 weeks
Frequency of treatm.	: daily
Duration of test	: up to 26 weeks
Doses	: 0.2%, 0.4%, 0.8% (n=30/sex/group)
Control group	: yes, concurrent no treatment
Method	: other: Directive 67/548/EEC, Part B and OECD Guideline 414
Year	:
GLP	: yes
Test substance	: other TS: 1,2-benzenedicarboxylic acid, Di-C8-C10 Branched Alkyl Esters, C9 Rich (CAS No. 68515-48-0)
Remark	: The potential reproductive toxicity of di-isononyl phthalate was assessed in one and two-generation reproductive toxicity studies. Groups of 30 male and female CRL:CD(SD)BR rats were given DINP via dietary administration at levels of either 0.0, 0.5, 1, or 1.5% (one generation study) or 0.0, 0.2, 0.4, or 0.8% (two generation study).

There were no changes in any of the classic reproductive parameters, i.e., mating, male or female fertility, fecundity, gestational index, or length of gestation in either study. The overall NOAELs for these effects were the highest dietary levels (%) tested ~ 500 mg/kg/day in the two generation study and 1000 mg/kg/day in the one-generation study. Adult survival was

unaffected at any level in either study.

Two-generation study:

In the two-generation study there were no testicular effects in either the P1 males, exposed as juveniles and young adults or the P2(F1) offspring exposed in utero, through lactation, and continuously to terminal sacrifice. The NOAEL was 470 mg/kg/day.

One-generation study:

Offspring survival was reduced at the 1.5% level (~ 1100 mg/kg/day) but unaffected at the 1% level (~ 760 mg/kg/day). Offspring body weights were decreased both at postnatal day (PND 0) and during lactation; however, the PND 0 effects were only clearly related to treatment at the 1.5% level. Weights of offspring during lactation were significantly reduced but within the historical control range at dietary levels (%) below 1%. As there was rapid recovery at the lower levels, even though treatment continued, the toxicologic significance is unclear. Weight gain was significantly reduced at the 1% level (~ 600 mg/kg/day). Liver and kidney weights were elevated at dietary level (%) above ~ 110 mg/kg/day, consistent with evidence from other studies of peroxisomal proliferation at these levels.

**Test substance** : 1,2-benzenedicarboxylic acid, Di-C8-C10 Branched Alkyl Esters, C9 Rich (CAS No. 68515-48-0)

**Conclusion** : This study showed that DINP treatment did not affect fertility or male reproductive development at doses of up to approximately 1000 mg/kg/day.  
07.12.2006 (11) (27)

## 5.9 SPECIFIC INVESTIGATIONS

### 5.10 EXPOSURE EXPERIENCE

### 5.11 ADDITIONAL REMARKS

**6.1 ANALYTICAL METHODS**

**6.2 DETECTION AND IDENTIFICATION**

**7.1 FUNCTION**

**7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED**

**7.3 ORGANISMS TO BE PROTECTED**

**7.4 USER**

**7.5 RESISTANCE**

**8.1 METHODS HANDLING AND STORING**

**8.2 FIRE GUIDANCE**

**8.3 EMERGENCY MEASURES**

**8.4 POSSIB. OF RENDERING SUBST. HARMLESS**

**8.5 WASTE MANAGEMENT**

**8.6 SIDE-EFFECTS DETECTION**

**8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER**

**8.8 REACTIVITY TOWARDS CONTAINER MATERIAL**



- (1) Barber E, Cifone M, Rundell J, Przygoda R, Astill B, Moran E, Mulholland A, Robinson E and Schneider B (2000). Results of the L5178Y mouse lymphoma assay and the Balb/3T3 cell in vitro transformation assay for eight phthalate esters. *Journal of Applied Toxicology* 20, 69-80.
- (2) Brown D, Croudace C, Williams N, Shearing J and Johnson P (1998). The effect of phthalate ester plasticisers tested as surfactant stabilised dispersions on the reproduction of the *Daphnia magna*. *Chemosphere* 36, 1367-1379.
- (3) Cousins I and Mackay D (2000). Correlating the physical-chemical properties of phthalate esters using the 'three solubility' approach. *Chemosphere* 41, 1389-1399.
- (4) EG & G Research Institute (1981). Evaluation of Test Article R-1218 (MRI #549) for Mutagenic Potential Employing the L5178Y TK+/- Mutagenesis Assay. Performed for Tenneco Chemicals. Final report. EPA Document No. 878210230.
- (5) EG&G Bionomics, Inc. (1983). Acute Toxicity of Fourteen Esters to Rainbow Trout *Salmo gairdneri* Under Flow-Through Conditions. Report No. BW-83-3-1373. Unpublished report.
- (6) Environmental Protection Agency (EPA) (2000). EPI Suite<sup>TM</sup>, Estimation Program Interface Suite, v3.12. U.S. EPA, Washington, DC, USA.
- (7) Exxon Biomedical Sciences, Inc. (1995). Ready Biodegradability, Manometric Respirometry. Study No. 199894A. Unpublished report.
- (8) Exxon Biomedical Sciences, Inc. (1996). In Vitro Chromosomal Aberration Assay in Chinese Hamster Ovary (CHO) Cells. Performed for Exxon Chemical Europe. Report date March, 1996. Unpublished report.
- (9) Exxon Biomedical Sciences, Inc. (1996). Microbial Mutagenesis in Salmonella Mammalian Microsome Plate Incorporation Assay. Performed for Exxon Chemical Europe. Report date March, 1996. Unpublished report.
- (10) Exxon Biomedical Sciences, Inc. (1996). Water Solubility. Report No. 199638. Exxon Biomedical Sciences, Inc., East Millstone, NJ, USA. Unpublished report.
- (11) Exxon Chemical (1996). Two Generation Reproduction Toxicity Study in Rats with Di-isononyl Phthalate (DINP). Final Laboratory Report. Unpublished report.
- (12) Hazleton Biotechnologies Co. (1986). Mutagenicity of 1J in a Mouse Lymphoma Mutation Assay - Final Report. Submitted to the Chemical Manufacturers Association. Report Date June, 1986.
- (13) Hazleton Laboratories, Inc. (1968). Acute Dermal Application - Rabbits. Report submitted to Exxon Research and Engineering Co. Report date May 20, 1968.
- (14) Hazleton Laboratories, Inc. (1968). Acute Oral Administration - Rats. Report submitted to Exxon Research and Engineering Co. Report date May 20, 1968.
- (15) Letinski D, Connelly M, Peterson D and Parkerton T (2002). Slow-stir water solubility measurements of selected alcohols and diesters. *Chemosphere* 48, 257-265.
- (16) Mackay D (1998). Level III Fugacity-Based Environmental Equilibrium Partitioning Model, Version 2.1 (16-bit). Environmental Modelling Centre, Trent University, Ontario, Canada.
- (17) McKee RH, Przygoda RT, Chirdon MA, Engelhardt G and Stanley M (2000). Di(isononyl) phthalate (DINP) and Di(isodecyl) phthalate (DIDP) are not mutagenic. *Journal of Applied Toxicology* 20, 491-497.

- (18) Patyna PJ, Parkerton TF, Davi RA, Brown RP, Letinski DJ, Thomas PE and Cooper KR (2001). Dietary Diisononyl phthalate (DINP) and Dissodecyl phthalate (DIDP) exposure in the Japanese Medaka (*Oryzias latipes*) multigeneration assay. Article accepted by Ecotoxicology and Environmental Safety, awaiting publication.
- (19) Rhodes J, Adams W, Biddinger G, Robillard K and Gorsuch J (1995). Chronic toxicity of 14 phthalate esters to *Daphnia magna* and Rainbow trout (*Oncorhynchus mykiss*). *Environ Toxicol Chem* 14, 1967-1976.
- (20) Springborn Bionomics, Inc. (1984). Acute Toxicity of Fourteen Esters to *Daphnia magna*. Report No. BW-84-4-1567. Unpublished report.
- (21) Springborn Bionomics, Inc. (1984). Acute Toxicity of Fourteen Esters to the Freshwater Green Alga *Selenastrum capricornutum*. Report No. BP-84-1-4. Unpublished report.
- (22) Springborn Bionomics. (1984). Chronic Toxicity Of Fourteen Phthalate Esters to *Daphnia magna*. Report No. BW-84-5-1567. Final Report Submitted to Chemical Manufacturers Association, Washington, DC, USA.
- (23) Staples C, Peterson D, Parkerton T and Adams W (1997). The environmental fate of phthalate esters: A literature review. *Chemosphere* 35, 667-749.
- (24) Staples CA, et al (1997). Aquatic toxicity of eighteen phthalate esters. *Environmental Toxicology and Chemistry* 16(5), 875-891.
- (25) Sugatt R, et al. (1983). Shake flask biodegradation of 14 commercial phthalate esters. Syracuse Research Corporation, Syracuse, NY, USA. SRC# L1543-05. Study performed for CMA (Chemical Manufacturers Association), Washington, DC, USA.
- (26) Waterman SJ, et al. (1999). Developmental toxicity of DIDP and DINP in rats. *Reproductive Toxicology* 13(2), 131-136.
- (27) Waterman SJ, et al. (1999). Two-generation reproduction study in rats given DINP in the diet. *Reproductive Toxicology* 14, 21-36.

## 10. Summary and Evaluation

Id 68515-48-0  
Date 07.12.2006

### 10.1 END POINT SUMMARY

### 10.2 HAZARD SUMMARY

### 10.3 RISK ASSESSMENT